L Number	Hits	Search Text	DB	Time stamp
1	35126	(mix$5 combin$7 react$4) same (sample specimen reagent chemical compound) and (422/$.ccls. or 436/$.ccls.)	USPAT; US-PGPUB	2003/09/04 09:29
2	6478	(mix$5 combin$7 react$4) same (sample specimen reagent chemical compound) and (422/$.ccls. or 436/$.ccls.) and computer	USPAT; US-PGPUB	2003/09/04 09:29
3	6163	(mix$5 combin$7 react$4) same (sample specimen reagent chemical compound) and (422/$.ccls. or 436/$.ccls.) and computer and (analy$6 detect$5)	USPAT; US-PGPUB	2003/09/04 09:30
4	4683	(mix$5 combin$7 react$4) same (sample specimen reagent chemical compound) same (analy$6 detect$5)and (422/$.ccls. or 436/$.ccls.) and computer	USPAT; US-PGPUB	2003/09/04 09:32
5	1948	((mix$5 combin$7 react$4) same (sample specimen reagent chemical compound) same (analy$6 detect$5)and (422/$.ccls. or 436/$.ccls.) and computer) not 422/$.ccls.	USPAT; US-PGPUB	2003/09/04 09:32
6	897	((mix$5 combin$7 react$4) same (sample specimen reagent chemical compound) same (analy$6 detect$5)and (422/$.ccls. or 436/$.ccls.) and computer) and (mass adj spectro$9)	USPAT; US-PGPUB	2003/09/04 09:41
7	73	((mix$5 combin$7 react$4) same (sample specimen reagent chemical compound) same (analy$6 detect$5)and (422/$.ccls. or 436/$.ccls.) and computer) and (mass adj spectro$9) and (deconvolut$5)	USPAT; US-PGPUB	2003/09/04 09:42

DOCUMENT-IDENTIFIER: US 20030049867 A1

TITLE: Methods for parallel detection of compositions having desired characteristics

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Current US Classification, US Primary Class/Subclass - CCPR (1):

436/518

Summary of Invention Paragraph - BSTX (8):

[0006] The present invention relates to the surprising discovery that up to thousands of samples, e.g., cells, biological compositions, chemical reaction compositions, and the like, can be simultaneously assessed for the presence and/or quantity of metabolic compounds, cofactors, and chemical reaction products, as well as various ions, metals, side products and the like, using magnetic resonance imaging (MRI). To simultaneously perform MRI on a plurality of samples, a physical array comprising a plurality of sample compartments is placed within the magnetic field and analyzed. Imaging techniques are then used to correlate spectroscopic signals to a particular sample compartment, thus providing an assessment of each sample in the array. Thus the present invention provides methods and apparatuses for screening a plurality of samples. Applications of these screening methods include, but are not limited to, methods of identifying metabolic disorder genes and methods of identifying modulatory compounds for use in drug development.

Summary of Invention Paragraph - BSTX (10):

[0008] Performing MRI spectroscopy in the present invention typically comprises exciting atomic nuclei in the samples, thereby producing a plurality of signals. The signals are detected and images are generated from the signals. In one embodiment, the images are obtained by applying spiral-based k-space trajectories. The images generated correspond to the plurality of spatial locations. The images are analyzed for the presence of one or more selected chemical shifts that correspond to the selected property. The images and chemical shifts are then deconvoluted to provide the spatial location for each of the one or more samples having the selected property. Therefore, the plurality of samples is simultaneously screened for the selected property.

Summary of Invention Paragraph - BSTX (15):

[0013] The samples analyzed using the apparatus and methods of the present invention include, but are not limited to, a library of

biological or chemical compositions, such as a library of expression products or variant genes or a library of mutagenized cells. Such libraries are optionally generated by DNA shuffling, random mutagenesis, transposon mutagenesis, or combinatorial gene assembly. Gene libraries are optionally expressed to produce libraries of expression products. Alternatively, the plurality of samples comprises one or more of: a microbial cell culture, a mammalian cell culture, a cell biomass, a culture broth, an extract, a reaction mixture, a plant tissue sample, a fruit sample, a root sample, a tuber sample, and a plant seed.

Summary of Invention Paragraph - BSTX (22):

[0020] In another embodiment, the apparatus further comprises a detector operably coupled to the spectrometer. The detector detects signals generated by operation of the MRI spectrometer. A computer and software are optionally coupled to the apparatus for recording and analyzing data from the MRI spectrometer.

Detail Description Paragraph - DETX (22):

[0057] In MRI, a field gradient is also applied to the sample to provide spatial information, as described above. The field gradient is optionally a one-dimensional or a two dimensional magnetic field gradient. A one-dimensional field gradient is a variation with respect to one dimension and a two-dimensional field gradient is a variation with respect to two directions. The typical symbols for a magnetic field gradient in the x, y, and z directions are G.sub.x, G.sub.y and G.sub.z. For example, when a magnetic field gradient is applied to a physical array containing, e.g., 24 spatially separated sample compartments, each sample compartment experiences a different magnetic field, and therefore the protons of interest in that sample, e.g., the ethanol protons will exhibit different chemical shifts. The result is an NMR spectrum with more than one signal. The amplitude of the signal is proportional to the number of spins in a plane perpendicular to the gradient. This is called frequency encoding and is used to deconvolute the signal, thus providing the spatial location for each signal. Backprojecting is then optionally used to generate an image of the physical array.

Detail Description Paragraph - DETX (23):

[0058] Backprojecting is one of the simplest ways to provide an image in MRI. Other techniques are available, e.g., Fourier transform imaging, that are well known to those of skill in the art. In backprojecting, a one-dimensional field gradient is applied at several angles, and an NMR spectrum is recorded for each angle. Once recorded, the data can be deconvoluted or backprojected through space, e.g., using a computer. Fourier transform imaging is a more commonly used method of imaging in magnetic resonance. This technique

involves a phase encoding gradient, a slice selection gradient, and a frequency encoding gradient. The three gradients are used to produce an FID for each spatial location screened. The FIDs are then fourier transformed to provide frequency and location information, e.g., for each sample well in a physical array.

Detail Description Paragraph - DETX (30):

[0065] The images produced using the above methods are deconvoluted to provide information on the samples in the array. "Deconvoluting" refers to the process of correlating the images obtained from MRI with the various spatial locations in the array. Deconvolution in the present application comprises determining the position of each sample according to the physical map. Therefore, the deconvolution optionally involves providing a comparison between a marker sample compartment and the physical array. The deconvolution step provides an indication of which sample compartments comprise a signal, i.e., which sample compartments correspond to a sample containing the compound of interest. It further involves comparing the various signals and providing a signal level for each sample compartment and/or sample. It further involves quantifying the amount of a particular compound in a particular sample compartment by a determination of signal intensity in each sample compartment.

Detail Description Paragraph - DETX (36):

[0071] A magnetic resonance imaging spectrometer is typically used in the present invention to excite the nuclei of the samples, thus screening for a selected property. The spectrometer comprises a magnet, which magnet produces a magnetic field (B) used for imaging. The magnet used in an MRI spectrometer is typically a superconducting magnet, which typically produces a magnetic field strength of about 1 Tesla to about 12 Tesla. Preferably the field strength comprises about 1 Tesla to about 5 Tesla, more preferably about 1.5 Tesla to about 3 Tesla. The magnet also typically comprises gradient coils that produce a gradient in magnetic field B, e.g., in the x, y, and z directions. Within the gradient coils is an rf coil. The rf coil produces a B.sub.1 field used to rotate the nuclei spins or net magnetization, e.g., by 45.degree., 90.degree., or 180.degree.. The rf coil is also used to detect a signal from the spins. For example, the rf coils detect the transverse magnetization as it precesses in the xy plane. The detector used is typically a quadrature detector that separates out M.sub.x and M.sub.y signals from the rf coil. MRI spectrometers are available from a variety of manufacturers, e.g., GE, which makes the GE SIGNA 1.5 Tesla imager. A schematic of a spectrometer is shown in FIG. 1. Magnet 100, gradient coil 102, and rf coil 104 surround physical array 114, thus placing physical array 114 within the magnetic field produced by magnet 100. The physical array is also susceptible to the gradient and rf radiation applied across the magnetic filed. The physical arrays and methods of the

present invention are optionally used with conventional MRI equipment using various data handling and representation software systems. Thus, the spectrometer, i.e., magnet 100, rf coil 104, and gradient coil 102, is typically coupled to computer 108, rf source 110, rf amplifier, 112, and rf detector 106.

Detail Description Paragraph - DETX (37):

[0072] A computer coupled to a spectrometer of the invention typically controls various components of the spectrometer. For example, the computer controls rf components, e.g., the radio frequency source, a pulse programmer, an amplifier, and the like. The rf source produces, e.g., a sine wave of the desired frequency, e.g., the resonant or Larmor frequency. A pulse programmer shapes the rf pulses, e.g., into apodized sine pulses. In addition, an rf amplifier is optionally used to increase pulse power, e.g., from milliwatts to kilowatts. The computer also optionally controls a gradient pulse programmer which sets the shape and amplitude of the gradient magnetic fields. An additional component is optionally an array processor, which is a device used to perform fast fourier transforms.

Detail Description Paragraph - DETX (38):

[0073] The computer, which optionally comprises an appropriately programmed processor, computer, or computer readable medium, is typically operably coupled to the MRI spectrometer and/or physical array and functions to instruct the operation of the apparatus of the invention, e.g., an MRI spectrometer, and its component elements in accordance with preprogrammed or user input instructions. The computer, processor, or other computer readable medium also optionally receives data and information from these instruments and interprets, manipulates, and reports this information to the user. As such, the computer is typically also appropriately coupled to one or more of: library storage elements, analog to digital or digital to analog control elements, and array processors, and the like.

Detail Description Paragraph - DETX (39):

[0074] The computer also typically includes appropriate software for receiving user instructions, e.g., in the form of user input into a set of parameter fields, e.g., in the form of preprogrammed instructions, e.g., preprogrammed for a variety of different specific operations. The software then converts these instructions to appropriate language for instructing movement of the physical array or control of the MRI spectrometer, and the like. The computer then receives data from one or more signal sensor/detectors included within the spectrometer system, and interprets the data, providing it in a user interpretable format, e.g., an image of each layer of the physical array, or using the data to initiate further instructions, such as in monitoring and control of sample rates, temperature,

applied field and the like.

Detail Description Paragraph - DETX (40):

[0075] In the present invention, the computer typically includes software for acquiring magnetic resonance data, monitoring of materials in the MRI spectrometer, and deconvolution of the data to provide an image of the array. Additionally the software is optionally used to control insertion and placement of the physical array within the spectrometer.

Detail Description Paragraph - DETX (41):

[0076] Typically, a computer commonly used to transform signals from the detection device into, e.g., concentrations will be a PC-compatible computer (e.g., having a central processing unit (CPU) compatible with x86 CPUs (e.g., a Pentium I, II or II class machine), and running an operating system such as, DOS.TM., OS/2 Warp.TM., WINDOWS/NT.TM., WINDOWS/NT.TM. workstation, or WINDOWS 98.TM.), or a Macintosh.TM. (running MacOS.TM.), or a UNIX workstation (e.g., a SUN.TM.workstation running a version of the Solaris.TM. operating system, a PC running LINUX, a PowerPC.TM. workstation or a mainframe computer), all of which are commercially common, and known to one of skill in the art. Data analysis software on the computer is then employed to deconvolute signal information. Software for these purposes is available, or can easily be constructed by one of skill using a standard programming language such as Visual Basic, Fortran, Basic, Java, or the like.

Detail Description Paragraph - DETX (42):

[0077] One of skill will immediately recognize that any, or all, of these components are optionally manufactured in separable modular units, and assembled to form an apparatus or system of the invention. Computers, rf coils, gradient coils, detectors, sample manipulation robots, and the like are optionally manufactured in a single unit, but more commonly are constructed as separate modules which are assembled to form an apparatus or system for analyzing a plurality of samples. Further, a computer does not have to be physically associated with the rest of the apparatus to be "operably linked" to the apparatus. A computer is operably linked when data is delivered from other components of the apparatus to the computer. One of skill will recognize that operable linkage can easily be achieved using either conductive cable coupled directly to the computer (e.g., USB, parallel, serial, ethernet, or phone line cables), or using data recorders which store data to computer readable media (typically magnetic or optical storage media such as computer disks and diskettes, CDs, magnetic tapes, but also optionally including physical media such as punch cards, vinyl media or the like) which is then accessed by the computer.

Detail Description Paragraph - DETX (43):

[0078] In traditional MRI, a patient is positioned within the magnetic field created by the magnet. The patient is typically placed on a table and positioned within a cavity within the magnet bore. For example, a patient is positioned on a computer controlled patient table that properly positions the patient within the magnetic field. In the present invention, the subject of the invention is a sample container or physical array containing samples to be screened, rather than a patient. The physical array is placed within the magnetic field or, alternatively, the magnetic field is applied to the plurality of samples. The arrays of the present invention are typically detectably coupled to, e.g., an MRI spectrometer during operation of the apparatus. "Detectably coupled" refers to placement of the array within the magnetic field of the spectrometer such that the samples within the array are excited and detected when performing MRI. Arrays useful in the present invention are described in more detail below.

Detail Description Paragraph - DETX (58):

[0093] The compound of interest in the present invention is often a component of a biological composition or a member of a library of biological compositions. Such biological compositions include, but are not limited to, microbial cell cultures, mammalian cell cultures, cell biomasses, culture broths, extracts, reaction mixtures, plant tissues, fruit samples, root samples, tuber samples, plant seeds, and the like. These compositions are optionally placed directly in the sample compartments of the physical array and screened directly for a compound of interest by performing MRI spectroscopy. Alternatively, a plurality of compositions is optionally purified, e.g., in an off-line parallel purification system. Examples of such systems have been developed by the inventors and their coworkers, e.g., for use in mass spectrometry systems, as in U.S. S No. 60/119,766 filed Feb. 11, 1999 and U.S. Ser. No. 09/502,283 filed Feb. 11, 2000, both entitled, "HIGH THROUGHPUT MASS SPECTROMETRY," which are incorporated herein by reference. The systems are optionally used for magnetic resonance samples in the same manner as described in No. 60/119,766 and Ser. No. 09/502,283. In other embodiments, the components of the biological compositions of interest are optionally purified and/or separated prior to MRI screening.

Detail Description Paragraph - DETX (78):

[0113] In silico methods of recombination can be effected in which genetic algorithms are used in a computer to recombine sequence strings which correspond to homologous (or even non-homologous) nucleic acids. The resulting recombined sequence strings are optionally converted into nucleic acids by synthesis of nucleic acids which correspond to the recombined sequences, e.g., in concert with

oligonucleotide synthesis/gene reassembly techniques. This approach can generate random, partially random or designed variants. Many details regarding in silico recombination, including the use of genetic algorithms, genetic operators and the like in computer systems, combined with generation of corresponding nucleic acids (and/or proteins), as well as combinations of designed nucleic acids and/or proteins (e.g., based on cross-over site selection) as well as designed, pseudo-random or random recombination methods are described in "METHODS FOR MAKING CHARACTER STRINGS, POLYNUCLEOTIDES & POLYPEPTIDES HAVING DESIRED CHARACTERISTICS" by Selifonov et al., filed Jan. 18, 2000, (PCT/US00/01202) "METHODS OF POPULATING DATA STRUCTURES FOR USE IN EVOLUTIONARY SIMULATIONS" by Selifonov and Stemmer (PCT/US00/01138), filed Jan. 18, 2000; and, e.g., "METHODS FOR MAKING CHARACTER STRINGS, POLYNUCLEOTIDES & POLYPEPTIDES HAVING DESIRED CHARACTERISTICS" by Selifonov et al., filed Jul. 18, 2000 (U.S. Ser. No. 09/618,579). Extensive details regarding in silico recombination methods are found in these applications.

Detail Description Paragraph - DETX (94):

[0129] Libraries can be biased towards nucleic acids which encode proteins with desirable enzyme activities. For example, after identifying a clone from a library which exhibits a specified activity, the clone can be mutagenized using any known method for introducing DNA alterations. A library comprising the mutagenized homologues is then screened for a desired activity, which can be the same as or different from the initially specified activity. An example of such a procedure is proposed in Short (1999) U.S. Pat. No. 5,939,250 for "PRODUCTION OF ENZYMES HAVING DESIRED ACTIVITIES BY MUTAGENESIS." Desired activities can be identified by any method known in the art. For example, WO 99/10539 proposes that gene libraries can be screened by combining extracts from the gene library with components obtained from metabolically rich cells and identifying combinations which exhibit the desired activity. It has also been proposed (e.g., WO 98/58085) that clones with desired activities can be identified by inserting bioactive substrates into samples of the library, and detecting bioactive fluorescence corresponding to the product of a desired activity using a fluorescent analyzer, e.g., a flow cytometry device, a CCD, a fluorometer, or a spectrophotometer.

Detail Description Paragraph - DETX (102):

[0137] Alternative libraries of the invention comprise chemical libraries or libraries of chemical compositions, such as a library of potential modulatory compounds. Essentially any chemical compound can be used as a potential modulator or library member in the screening assays of the invention, although most often compounds can be dissolved in aqueous solutions, organic (especially DMSO-based) solutions are also used. Alternatively, a library or group of solid

phase compositions is screened or assayed. It will be appreciated that there are many suppliers of chemical compounds, including Sigma (St. Louis, Mo.), Aldrich (St. Louis, Mo.), Sigma-Aldrich (St. Louis, Mo.), Fluka Chemika-Biochemica Analytika (Buchs Switzerland), and the like. In one preferred embodiment, high throughput screening methods involve providing a combinatorial library containing a large number of potential therapeutic compounds (potential modulator compounds). Such combinatorial chemical libraries are then screened in one or more assays to identify those library members (particular chemical species or subclasses) that display a desired characteristic property, such as modulators that alleviate, e.g., reduction of metabolite levels related to a metabolic disorder. The compounds thus identified can serve as conventional "lead compounds" or can themselves be used as potential or actual therapeutics.

Detail Description Paragraph - DETX (137):

[0172] The methods of identifying a catalyst include (i) providing a plurality of assay solutions, which plurality of assay solutions comprises at least one reactant; (ii) providing a plurality of catalysts (iii) combining the plurality of assay solutions and the plurality of catalysts; (iv) performing magnetic resonance (MRI) spectroscopy on the plurality of assay solutions, thereby detecting one or more products generated by an action of the catalyst on the at least one reactant; and (v) identifying one or more of the plurality of catalysts that alter the level of the at least one of the one or more products, thereby identifying a catalyst. At least one member of the plurality of catalysts is added to the plurality of assay solutions. Optionally, the plurality of catalysts are omitted from at least one assay solution, such that the assay solution can be used as a control assay solution. The plurality of catalysts optionally comprises cells, cellular extracts, or media collected from cell cultures. Alternatively, the plurality of catalysts comprises a library of synthesized or isolated compounds, such as a combinatorial library of compounds.

Detail Description Paragraph - DETX (139):

[0174] Other factors that can be varied within the assay solution composition include the ratio of water to organic solvent(s); the presence of organic and/or inorganic ions; the presence and pressure of oxygen or other gases; and the presence of catalyst activators or deactivators, or other chemical compounds (for example, plasticizers) that can otherwise influence the progression of the chemical reaction. Environmental factors that can be varied include temperature, pressure, electromagnetic radiation, ultrasound or other radiofrequencies, and the like. For reactions involving catalysis of polymers; the compositions of the co-monomers for polymer synthesis, or composition of polymers for polymer modification or depolymerization reactions, can be varied and/or optimized. In

addition, the structure of the reactant is optionally varied. A library of compounds, or a plurality of reactants is optionally provided, the members of which comprise structural variants of one or more compounds for which a desired chemical conversion is sought (for example, one or more compound sets can be provided, where each set is represented by various olefins, carboxylic acids, alcohols, phenols, amines and the like, such as those used in catalyst specificity analysis or in combinatorial chemistry).

Detail Description Paragraph - DETX (140):

[0175] The method of optimizing can further include determining a "window of operation" of a catalyst. Determining this window is accomplished, for example, by analyzing the factors (i.e., reaction parameters) that limited or expanded the performance of the catalyst in the assay solution. This analysis provides sets of ranges of the different reaction parameters over suitable operation conditions for the given catalyst. Optionally, the conditions influencing performance of a given catalyst are further examined and optimized within such a window of operation, by iterative application of the methods of the present invention. Additional arrays of samples or assay solutions are optionally exposed to reaction parameters set within more narrowly defined boundaries than that of the preceding set of assay solutions, to determine optimal conditions within the previously established window of operation. Thus, the performance of a given catalyst under varying reaction conditions is optionally determined using the methods of the present invention, providing information regarding the efficiency of the catalyst and optimization of the catalyzed reaction.

Claims Text - CLTX (3):

2. The method of claim 1, wherein each member of the plurality of samples comprises one or more atomic nuclei and the performing MRI comprises: (a) exciting the one or more atomic nuclei, thereby producing a plurality of signals; (b) detecting the plurality of signals; (c) generating one or more images from the plurality of signals, which one or more images correspond to the plurality of spatial locations; (d) analyzing the one or more images for the presence of one or more selected chemical shifts; which one or more selected chemical shifts correspond to the selected property; and, (e) deconvoluting the one or more images and the one or more selected chemical shifts to provide the spatial location for each of the one or more samples having the selected property, thereby screening the plurality of samples for the selected property.

Claims Text - CLTX (62):

61. The apparatus of claim 45, further comprising a computer and software operably coupled to the apparatus for recording and

analyzing data from the magnetic resonance imaging spectrometer.

Claims Text - CLTX (91):

90. The method of claim 89, wherein step (c) comprises: (d) exciting one or more atomic nuclei in the one or more metabolites, thereby producing a plurality of signals; (e) detecting the plurality of signals; (f) generating one or more images from the plurality of signals, which one or more images correspond to the plurality of spatial locations; (g) analyzing the one or more images for the presence of one or more selected chemical shifts; which one or more selected chemical shifts correspond to the one or more metabolites; and, (h) deconvoluting the one or more images and the one or more selected chemical shifts to provide the spatial location for each of the one or more cells having the one or more metabolites.

Claims Text - CLTX (113):

112. The method of claim 107, wherein identifying one or more of the plurality of potential chemical catalysts that alter the level of the at least one of the one or more products comprises analyzing product yields, compositions, reaction selectivity, catalyst stability, catalyst poisoning, or combinations thereof.

TI Oxygen binding to partially oxidized hemoglobin. Analysis in terms of an allosteric model

AU Cordone, Lorenzo; Cupane, Antonio; Leone, Maurizio; Militello, Valeria; Vitrano, Eugenio

CS Ist. Fis., Univ. Palermo, Palermo, 90123, Italy

SO Biophysical Chemistry (1990), 37(1-3), 171-81
CODEN: BICIAZ; ISSN: 0301-4622

DT Journal

LA English

AB Oxygen binding to partially oxidized (aquomet) Hb is studied. The fractional satn. with oxygen is evaluated by **deconvoluting** the optical absorption **spectra**, in the 500-700 nm wavelength region, in terms of oxyHb, deoxyHb, and metHb spectral components. Expts. have been performed with auto-oxidized **samples** and with **samples** obtained by **mixing** ferrous Hb with fully oxidized Hb (**mixed samples**). An increase in oxygen affinity and a decrease in cooperativity are obsd. on increasing the amt. of ferric Hb in the sample. A high cooperativity (nH ~2) is maintained even in the presence of 50-60% ferric hemes. Moreover, for equal amts. of metHb the oxygen affinity is lower and the cooperativity higher for **mixed samples** than for those auto-oxidized. The results are analyzed within the framework of a modified Monod-Wyman-Changeux allosteric model taking into account the effects brought about by the presence of oxidized hemes and of αβ dimers. The distribution of ferric subunits within the tetramers in fully deoxygenated and fully oxygenated samples, as derived from the model, provides details on the cooperative behavior of partially oxidized Hb.

L6 ANSWER 22 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text

AN 112:148338 CA

TI **Hadamard** transform measurement of tandem Fourier-transform mass spectra

AU Williams, Evan R.; Loh, Stanton Y.; McLafferty, Fred W.; Cody, Robert B.

CS Chem. Dep., Cornell Univ., Ithaca, NY, 14853-1301, USA

SO Analytical Chemistry (1990), 62(7), 698-703
CODEN: ANCHAM; ISSN: 0003-2700

DT Journal

LA English

AB The simultaneous collection of multiple spectra using tandem (MS/MS) and multidimensional (MS/MS/MS) mass spectrometry from multiple precursors yields correspondingly enhanced sensitivity. This approach uses **Hadamard** transform **deconvolution** and takes advantage of the multichannel dissocn. capability of Fourier-transform mass spectrometry. By application of this this to an 11-component mixt., the 11 spectra of the products of dissocg. 11 different combinations of 6 of the component mol. ions were measured; **Hadamard** transformation yields individual spectra of the precursor ions exhibiting a signal-to-noise improvement of 1.8 times over the spectra measured sep., as predicted by theory. Precursor ion selection with high specificity and product formation with high abundance reproducibility are crit.; spurious peaks resulting from imperfect reproducibility can be minimized by using simultaneous equation coeffs. reflecting the degree of precursor dissocn. Extension of this technique is demonstrated with simultaneous MS/MS/MS monitoring of three precursors and three daughters yielding nine spectra representing the 9 possible dissocn. pathways. Coding the product relationships for each addnl. step (e.g., precursor → daughter, daughter → granddaughter) requires elimination of half of the remaining ions. No ions are lost for coding in an improved **Hadamard** approach in which the combined daughter spectrum of the selected half of the precursors is subtracted from that of the other half.

L6 ANSWER 23 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 108:176472 CA
TI On the use and the performance of the delta function convolution method for the estimation of fluorescence decay parameters
AU Boens, N.; Ameloot, M.; Yamazaki, I.; De Schryver, F. C.
CS Dep. Chem., Kathol. Univ., Lovain, B-3030, Belg.
SO Chemical Physics (1988), 121(1), 73-86
CODEN: CMPHC2; ISSN: 0301-0104
DT Journal
LA English
AB The delta function convolution method (DFCM) is a rigorous and convenient procedure for the anal. of time-correlated single photon counting expts. DFCM **deconvolutes** the **sample** decay by the decay of a monoexponential ref. compd. to circumvent the wavelength dependence of the instrument. The accuracy of the parameter recovery by DFCM was investigated in a systematic way on simulated data sets. Mono- and biexponential **sample** decays are considered in **combination** with different ref. lifetimes. The effect on the parameter recovery when a multiexponentially decaying ref. is erroneously taken at being monoexponential is discussed. The formula for DFCM using a multiexponential ref. were derived. Recursion formulas for a computer anal. program in the case of a (multi-)exponential sample decay and a monoexponential ref. are provided.

L6 ANSWER 24 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 96:7288 CA
TI Structure of polyethylene solid solutions. 2. Aspects of spectral deconvolution
AU Burchell, D. J.; Hsu, S. L.
CS Dep. Polym. Sci. Eng., Univ. Massachusetts, Amherst, MA, 01003, USA
SO Polymer (1981), 22(7), 907-11
CODEN: POLMAG; ISSN: 0032-3861
DT Journal
LA English
AB Four methods of factor anal. were evaluated and applied to **deconvolution** of the IR **spectra** for solid solns. of binary **mixts**. of polyethylene [9002-88-4] **samples** having .hivin.Mn 980 and 1790, resp. In addn. to the cryst. orthorhombic form, these spectroscopic techniques revealed a packing disorder in the form of a monoclinic phase. This can be correlated with the amt. of conformational disorder assocd. with the samples.

L6 ANSWER 25 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 81:84048 CA
TI Application of the **Hadamard** transform to NMR spectrometry with pseudonoise excitation
AU Kaiser, Reinhold
CS Dep. Phys., Univ. New Brunswick, Fredericton, NB, Can.
SO Journal of Magnetic Resonance (1969-1992) (1974), 15(1), 44-63
CODEN: JOMRA4; ISSN: 0022-2364
DT Journal
LA English
AB The multichannel method of measuring a set of independent sample values of a phys. variable is discussed with ref. to high-resoln. NMR spectrometry, and the achievable signal/noise gain is formulated. A multichannel measurement of the free induction decay is considered, and the use of input signals derived from max.-length binary pseudorandom sequences offers certain computational advantages. In particular, the relation

between these sequences and **Hadamard** matrixes is explored, and a fast algorithm for the **deconvolution** of the output from such input signals is developed. The use of this method to measure the free induction decay and spectrum is illustrated with a simple example, and the limitation of the achievable signal/noise gain, due to satn. of the spin system, is considered.

=> log y

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STN INTERNATIONAL LOGOFF AT 16:28:25 ON 28 AUG 2003

immediate-release formulation used as control and that the release rate, although close to the desired value, lasts only 7 or 8 h; these results agree with those given by numerical **deconvolution** using the mean urinary excretion curves.

L6 ANSWER 19 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 115:169510 CA
TI Distribution of event times in time-resolved fluorescence: the exponential series approach - algorithm, regularization, analysis
AU Landl, Gerhard; Langthaler, Thomas; Engl, Heinz W.; Kauffmann, Harald F.
CS Inst. Phys. Chem., Univ. Wien, Vienna, A-1090, Austria
SO Journal of Computational Physics (1991), 95(1), 1-28
CODEN: JCTPAH; ISSN: 0021-9991
DT Journal
LA English
AB In time-resolved fluorescence spectroscopy, a distribution of fluorescence lifetimes resulting from static and dynamic disorder of a polychromophoric ensemble is to be detd. from the mol. fluorescence response to the optical probe pulse. To do this, one has to solve a convolution integral equation of the first kind and then invert a Laplace transform. Both problems are ill-posed in the sense of **Hadamard**. An algorithm that combines coarse discretization for inverting the Laplace transform with a nonlinear least-squares approach based on Newton and quasi-Newton techniques for solving the convolution equation. While this algorithm works well in many cases, it does not completely remove the instabilities due to the ill-posedness. Thus, also proposed is an algorithm that combines the approach described above with Tikhonov regularization. Several examples, both with synthetic and with real data, show the performance of the algorithms.

L6 ANSWER 20 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 114:153737 CA
TI **Hadamard** transform measurement of multidimensional (MSn) Fourier-transform mass spectra
IN Williams, Evan R.; McLafferty, Fred W.
PA Cornell Research Foundation, Inc., USA
SO U.S., 18 pp. Cont.-in-part of U.S. 4,931,639.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4978852	A	19901218	US 1990-500483	19900328
	US 4931639	A	19900605	US 1988-241869	19880908
PRAI	US 1988-241869		19880908		
	US 1988-239423		19880901		

AB The simultaneous collection of multiple spectra using tandem and multidimensional mass spectrometry from multiple precursors yields correspondingly enhanced sensitivity through **Hadamard** transform **deconvolution**. For MSn spectra, the product relationships are coded by a **Hadamard** differences method wherein the combined daughter spectrum of a selected half of the precursors is subtracted from the combined daughter spectrum of the remaining precursors, so that no ions are lost.

L6 ANSWER 21 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 113:226629 CA

that these exponential functions are notoriously difficult to approx. with a Marquardt-Levenberg algorithm, the validity of the results may be questionable. Three examples (protonated benzene, cycloheptatriene, deuterated toluene) are chosen to demonstrate some of the difficulties and pitfalls of the procedure.

L6 ANSWER 17 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 119:31231 CA
TI Fourier transform infrared **Hadamard** tomography of sooting flames
AU Bates, Stephen C.; Carangelo, Robert; Knight, Kim; Serio, Michael
CS Adv. Fuel Res., East Hartford, CT, 06108, USA
SO Review of Scientific Instruments (1993), 64(5), 1213-21
CODEN: RSINAK; ISSN: 0034-6748
DT Journal
LA English
AB An exptl. technique was described that combines tomog., **Hadamard** signal encodement, and a patented Fourier-transform IR (FT-IR) emission-transmission technique to perform simultaneous spatially resolved gas species and soot measurements during combustion. Tomog. anal. of line-of-sight FTIR data allowed spatially resolved measurements to be made. **Hadamard** encodement of the tomog. sections increased the overall signal throughput and improved the signal-to-noise (S/N) ratio for each measurement. Use of the **Hadamard** technique resulted in a major simplification in the tomog. app. in that the scanning app. that would normally by required was eliminated, and focusing of the IR light was much easier. **Deconvolution** of the encoded data was accurate and gave the predicted improvement in S/N ratio. FT-IR **Hadamard** tomog. was performed to measure soot in a fuel-rich ethylene diffusion flame. Spatially resolved concn. measurements agreed well with previous data and clearly showed striking 3-dimensional features that could not normally be measured by simple line-of-sight techniques.

L6 ANSWER 18 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 116:11131 CA
TI Design and evaluation of sustained-release tablets of lithium in a fat matrix and its bioavailability in humans
AU Llabres, M.; Farina, J. B.
CS Fac. Farm., Univ. La Laguna, La Laguna, 38200, Spain
SO Journal of Pharmaceutical Sciences (1991), 80(11), 1012-16
CODEN: JPMSAE; ISSN: 0022-3549
DT Journal
LA English
AB The development of sustained-release lithium (Li) tablets, intended to release the active principle at a rate of 1.0 mM/h for 10 h, was undertaken. The parameters used for the control of the release were the glyceryl palmite-stearate content, the carboxypolymethylene content, and the compression force. The exptl. design is based on **Hadamard**'s matrixes and is of the adaptation by stages type. The formulation seen as optimal from in vitro assays was later assessed in vivo by a crossover study of six subjects. The parameters used to measure the bioavailability were the total amt. of Li excreted in the urine in the 96 h following ingestion, the max. urinary excretion rate, and the time at which this rate was reached. The acceptability interval for the first two parameters was established from the theor. curve of urinary excretion, which was calcd. by convolution of the desired in vivo release variable (1.0 mM/h for 10 h) by the absorption-disposition variable obtained after administering the prepn. in Li carbonate capsules. The results obtained show that the bioavailability of the formulation is 75% of the

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=> d his

     (FILE 'HOME' ENTERED AT 16:20:45 ON 28 AUG 2003)
     FILE 'CA' ENTERED AT 16:20:54 ON 28 AUG 2003
L1           454 S HADAMARD
L2            13 S L1 AND DECONVOL?
L3          1825 S DECONVOL?(4A)(SAMPLE OR SPECTRUM OR MIXTURE)
L4         38524 S (MIX? OR COMBIN?)(7A)(SAMPLE OR SPECIMEN)
L5            12 S L3 AND L4
L6            25 S L2,L5

=> d bib,ab 1-25 l6

L6   ANSWER 1 OF 25  CA  COPYRIGHT 2003 ACS on STN
Full Text
AN   139:28131  CA
TI   Effects of modulation defects on Hadamard transform time-of-flight mass
     spectrometry (HT-TOFMS)
AU   Kimmel, Joel R.; Fernandez, Facundo M.; Zare, Richard N.
CS   Department of Chemistry, Stanford University, Stanford, CA, USA
SO   Journal of the American Society for Mass Spectrometry (2003), 14(3),
     278-286
     CODEN: JAMSEF; ISSN: 1044-0305
PB   Elsevier Science Inc.
DT   Journal
LA   English
AB   In any Hadamard multiplexing technique, discrepancies between the
     intended and the applied encoding sequences may reduce the intensity of
     real spectral features and create discrete, artificial signals.  In
     implementation of Hadamard transform time-of-flight mass spectrometry
     (HT-TOFMS), the encoding sequence is applied to the ion beam by an
     interleaved comb of wires (Bradbury-Nielson gate), which shutters the ion
     beam on and off.  By isolating and exaggerating individual skewing effects
     in simulating the HT-TOFMS process, the authors detd. the nature of errors
     that arise from various defects.  In particular, the most damaging defects
     are: mismatched voltages between the wire sets and the acceleration
     voltage of the instrument, which cause pos. and neg. peaks throughout mass
     spectra; insufficient deflection voltage, which reduces the intensity of
     real peaks and causes neg. peaks that are spread across the entire mass
     range; and voltage errors as the wire sets return from their deflection
     voltage to their transmission value, which yield significant redns. in
     peak intensities, create artificial peaks throughout mass spectra, and
     broaden real peaks by causing pos. peaks to grow in the bins adjacent to
     them.  Because the magnitude of the modulation defects grows as the
     applied modulation voltage is increased, Bradbury-Nielson gates with finer
     wire spacing, and hence stronger effective fields for a given applied
     voltage, were produced and installed.  Operating at 10 to 15 V where
     errors in the electronics are essentially absent, the most finely spaced
     gate (100 μm) yielded signal-to-noise ratios that were >2 times higher
     than those achieved with more widely spaced gates.  As an alternative
     method for minimizing skewing effects, HT-TOFMS data were post processed
     using an exact knowledge of the modulation defects.  Nonbinary matrixes
     that mimic the actual encoding process were built by measuring voltage vs.
     time traces and then translating these traces to transmission vs. time.
     Use of these matrixes in the deconvolution step led to marked
     improvements in spectral resoln. but require full knowledge of the
     encoding defects.
RE.CNT  20    THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
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L6 ANSWER 2 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 135:93304 CA
TI NMR Measurements Related to Clay-Dispersion Quality and Organic-Modifier Stability in Nylon-6/Clay Nanocomposites
AU VanderHart, D. L.; Asano, A.; Gilman, J. W.
CS Polymers Division, National Institute of Standards and Technology, Gaithersburg, MD, 20899, USA
SO Macromolecules (2001), 34(12), 3819-3822
CODEN: MAMOBX; ISSN: 0024-9297
PB American Chemical Society
DT Journal
LA English
AB Solid-state NMR was used to study the quality of clay dispersion and the stability of org. modifiers in nylon-6 (N6)/clay nanocomposites produced by various processing conditions, from longitudinal relaxation (T1H) data. The org. modifiers on clay pellets are di-Me dihydrogenated-tallow quaternary ammonium chloride or bis(2-hydroxyethyl) ammonium chloride and the polyamide used is Capron B135WP. The components were **mixed**, heated, and slowly cooled by compaction; the **samples** were produced by machining into 3 mm o.d. cylinders. The **deconvoluted** 75 MHz 13C CPMAS **spectra** of the CR region of the nanocomposites show strong contrast in the line width of the cryst. (CR) and non-cryst. (NC) signals of slowly cooled N6-SC, where the superior order and rigidity of the CR lattice results in sharper lines. The CR signals for N6-SC and the nanocomposite are very different and correspond to the published spectra of the α- and γ-cryst. forms. Data indicate that degrdn. of org. modifiers is directly related to better dispersion of clay in the nanocomposites.
RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 135:51724 CA
TI The use of modulated temperature programs in thermal methods
AU Reading, M.
CS IPTME, Loughborough University, Loughborough, LE11 3TU, UK
SO Journal of Thermal Analysis and Calorimetry (2001), 64(1), 7-14
CODEN: JTACF7; ISSN: 1418-2874
PB Kluwer Academic Publishers
DT Journal; General Review
LA English
AB A review with 41 refs. is presented. Temp. modulation has long been used in various aspects of thermal methods. Historically, the principle areas of application have been the detn. of kinetic parameters using variants of the temp. jump method and the measurement of heat capacity by AC calorimetry. More recently the introduction of temp. modulation in a variety of techniques has been used in **combination** with **deconvolution** algorithms to sep. **sample** responses that are dependent on rate of change of temp. from those principally dependent on temp. Finally, temp. modulation is important in the new field of microthermal anal.
RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 134:258759 CA
TI New deconvolution method for electrospray ionization mass spectrometry
AU Kato, Hiroshi; Ishihara, Morio; Nakata, Munetaka
CS JEOL Ltd., Akishima, Tokyo, 196-8558, Japan

SO Journal of the Mass Spectrometry Society of Japan (2000), 48(6), 373-379
CODEN: JMSJEY; ISSN: 1340-8097
PB Nippon Shitsuryo Bunseki Gakkai
DT Journal
LA English
AB A new method is proposed for elimination of artifacts appearing in **deconvolution** of electrospray ionization mass **spectra**, where two algorithms, a partial correlation method (PCM) and a sub-harmonic artifact removal filter (SHARF), are used. In addn. to the elimination of artifacts, the former algorithm removes influence of singly charged ions generated from contamination in a sample, while the latter algorithm removes influence of background noises and baseline offsets in a measured spectrum. The proposed method results in supplying the **deconvoluted spectra** free from artifacts with good signal-to-noise ratios and without distortion on peak shapes. Applications to some bio-mols. lead to the conclusion that our method is esp. useful for analyses of their **mixt. samples**, which show complicated mass spectra.
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 133:131683 CA
TI Moessbauer and EPR Characterization of the S = 9/2 Mixed-Valence Fe(II)Fe(III) Cluster in the Cryoreduced R2 Subunit of Escherichia coli Ribonucleotide Reductase
AU Krebs, Carsten; Davydov, Roman; Baldwin, Jeff; Hoffman, Brian M.; Bollinger, J. Martin, Jr.; Huynh, Boi Hanh
CS Department of Physics Rollins Research Center, Emory University, Atlanta, GA, 30322, USA
SO Journal of the American Chemical Society (2000), 122(22), 5327-5336
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB Low-temp. (77 K) radiolytic redn. of the diferric cluster in the met R2 subunit of Escherichia coli ribonucleotide reductase yields an antiferromagnetically coupled mixed-valence Fe(II)Fe(III) cluster ([R2met]mv1/2). Annealing the radiolytically reduced **sample** at 180 K converts the **mixed**-valence cluster in [R2met]mv1/2 into a ferromagnetically coupled cluster having an S = 9/2 ground state (R2mv9/2). We have used Moessbauer and EPR spectroscopy to study the electronic and magnetic properties of R2mv9/2. The Moessbauer data, recorded over wide ranges of temp. and applied field, indicate that the mixed-valence cluster in R2mv9/2 is valence localized. The **spectra** can be **deconvoluted** into two spectral components, of which anal. yields parameters (δ = 1.25 mm/s, ΔEQ = -2.80 mm/s, η = 1.30, and a/gnβn = -(13.5, 10.8, 20.3) T for site 1; and δ = 0.53 mm/s, ΔEQ = -0.57 mm/s, η = -3, and a/gnβn = -(22.1, 22.0, 22.0) T for site 2) that are characteristic of high-spin ferrous (site 1) and high-spin ferric (site 2) ions with octahedral O/N coordination. The spin-spin interaction between the two valence localized iron sites is ferromagnetic and the effective exchange coupling const. (Jeff in the exchange Hamiltonian JeffS1•S2) is estd. to be ca. -12 cm-1 from the high-temp. strong-field data. Taking into consideration the various factors that control the electronic properties of a mixed-valence Fe(II)Fe(III) compd. and comparing the obsd. spectroscopic properties of R2mv9/2 with those of model complexes, a core structure with two single-oxygen bridges is proposed for R2mv9/2. It is suggested that

conversion of [R2met]mv1/2 to R2mv9/2 may involve a carboxylate shift of E238 from a monodentate terminal chelating mode to a monodentate bridging and chelating mode, in addn. to protonation of the oxo bridge. R2mv9/2 displays EPR signals at g = 14-15, 6.6, and 5.4. Anal. of the data indicates that these features can be properly simulated by assuming an S = 9/2 center with a central E/D of 0.05 and a distribution in E/D ($\sigma E/D = 0.023$). Effects of E/D distribution on the EPR spectrum are discussed.

RE.CNT 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 133:117081 CA
TI Three-dimensional spectral imaging by **Hadamard** transform spectroscopy in a programmable array microscope
AU Hanley, Q. S.; Verveer, P. J.; Arndt-Jovin, D. J.; Jovin, T. M.
CS Department of Molecular Biology, Max Planck Institute for Biophysical Chemistry, Gottingen, D-37077, Germany
SO Journal of Microscopy (Oxford) (2000), 197(1), 5-14
CODEN: JMICAR; ISSN: 0022-2720
PB Blackwell Science Ltd.
DT Journal
LA English
AB We report the acquisition and **deconvolution** of three-dimensional spectrally resolved images in a programmable array microscope implementing a **Hadamard** transform fluorescence spectroscopy system with adjustable spectral resoln. A stack of 16 two-dimensional spectral images was collected at 400 nm intervals along the optical axis. The specimen consisted of a polytene chromosome spread from Drosophila melanogaster doubly labeled for the Polyhomeotic protein by indirect immunofluorescence labeling with Alexa594 and for DNA with YOYO-1. The resulting four-dimensional data set consisted of the xyz spatial dimensions (898×255×16) with a 26-point spectrum at each spatial location. The total exposure time to the sample was 34 min. The system requires the acquisition of multiple images, and thus works best with fluorophores that are resistant to photobleaching. Image **deconvolution** reduced the amt. of out-of-focus blur by up to a factor of 8, resulting in a dramatic improvement in the visualization of the chromosome backbone and localization of the specific Polyhomeotic domains.

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 133:52820 CA
TI A multiple window deconvolution technique for measuring low-energy beta activity in samples contaminated with high-energy beta impurities using liquid scintillation spectrometry
AU Verrezen, F.; Hurtgen, C.
CS Low-Level Radioactivity Measurements, Department of Radioprotection, Belgian Nuclear Research Centre (SCK-CEN), Mol, B-2400, Belg.
SO Applied Radiation and Isotopes (2000), 53(1-2), 289-296
CODEN: ARISEF; ISSN: 0969-8043
PB Elsevier Science Ltd.
DT Journal
LA English
AB An optimized multiple window counting technique, using liq. scintillation counting combined with internal standardization and spectrum unfolding was developed for the assessment of low-level, low-energy beta activity in

multi-labeled samples contg. high-energy beta impurities. Distinct spectral contributions are reconstructed for every individual radionuclide and impurity using software deconvolution techniques. The most important advantages of this method are that it does not require setting up quench correction curves and that the exact knowledge of ref. activity is not required, thus eliminating two important sources of uncertainty in the final results. The technique was successfully used on mixts. of 3H, 14C, 63Ni, 99Tc and 60Co over a wide range of quenching and activity ratios.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 129:285333 CA
TI Determination of plutonium-240/239 ratios in low activity samples using high resolution alpha-spectrometry
AU La Mont, S. P.; Glover, S. E.; Filby, R. H.
CS Department Chemistry, Washington State University, Pullman, WA, 99164, USA
SO Journal of Radioanalytical and Nuclear Chemistry (1998), 234(1-2), 195-199
CODEN: JRNCDM; ISSN: 0236-5731
PB Elsevier Science S.A.
DT Journal
LA English
AB Isotopic ratios of 240Pu/239Pu in certified std. materials and std. biol. materials (human liver) were measured using a combination of high resoln. alpha-spectroscopy and spectrum anal. software. This method uses unmodified, com. available equipment and software. Pu alpha-spectra were gathered with an alpha-spectrometer system set up for low-level actinide detn. Exptl. spectra were imported into a data anal. program, and fitted with math. descriptions of alpha-peaks using the Marquardt-Levenberg algorithm. The **spectra** were then **deconvoluted** into its 239Pu and 240Pu components and the activity ratio was calcd.

L6 ANSWER 9 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 129:225103 CA
TI **Hadamard** transform time-of-flight mass spectrometry
AU Brock, Ansgar; Rodriguez, Nestor; Zare, Richard N.
CS Department of Chemistry, Stanford University, Stanford, CA, 94305, USA
SO Analytical Chemistry (1998), 70(18), 3735-3741
CODEN: ANCHAM; ISSN: 0003-2700
PB American Chemical Society
DT Journal
LA English
AB A new mode of operation of a time-of-flight mass spectrometer (TOFMS) is described and demonstrated. A continuous ion beam emerging from the ion source is accelerated and then modulated by a pseudorandom sequence of on and off pulses. The data acquisition period is set to match the period of the modulation sequence, and data are acquired synchronously with the modulation of the ion beam. The modulation sequence is **deconvoluted** from the data using a fast **Hadamard** transform (FHT) algorithm to ext. the time-of-flight distribution of the ions. This multiplexing scheme increases the ion usage to ~50% for a single detector instrument and ~100% for a multiple detector instrument, which improves the signal level considerably over that of conventional TOFMS. The gains in signal lead to an improved signal-to-noise ratio or alternatively reduced data acquisition time, giving HT-TOFMS a major instrumental advantage over conventional TOFMS in a no. of applications at little addnl. cost. Pos. mode electrospray ionization mass spectra of tetrabutylammonium perchlorate, cesium chloride, and a protein mixt. of cytochrome c and

ubiquitin are presented to illustrate the method and the device.
RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 126:81909 CA
TI A method for measuring the mobility spectra of ions with ion mobility spectrometers (IMS)
IN Franzen, Jochen
PA Bruker-Franzen Analytik Gmbh, Germany
SO Brit. UK Pat. Appl., 12 pp.
CODEN: BAXXDU
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 2300296	A1	19961030	GB 1996-8740	19960426
	GB 2300296	B2	19990609		
	DE 19515270	A1	19961107	DE 1995-19515270	19950426
	DE 19515270	C2	20000511		
	US 5719392	A	19980217	US 1996-637199	19960424
PRAI	DE 1995-19515270		19950426		

AB The title methods entail impressing upon the essentially continuous ion flow of an IMS ion source, which comprises various ion types with various mobilities, a temporal switching pattern by using a very fast ion flow switch. From the Quasi-continuously received ion current signal at the end of the path of the ion mobility spectrometer the compn. of the ion types can be recovered according to mobility and intensity by math. **deconvolution** (e.g., using a **Hadamard** or Fourier transform). The methods allow a high duty cycle (e.g., about 50%). Spectrometers provided with switching and detection means for carrying out the methods are also described. Application to air pollution monitoring is indicated.

L6 ANSWER 11 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 124:32962 CA
TI FTIR study of ultradispersed diamond powder synthesized by explosive detonation
AU Jiang, T.; Xu, K.
CS Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, Lanzhou, 730000, Peop. Rep. China
SO Carbon (1995), 33(12), 1663-71
CODEN: CRBNAH; ISSN: 0008-6223
PB Elsevier
DT Journal
LA English
AB Ultradispersed diamond (UDD) powders synthesized by explosive detonation were studied by FTIR to explore their surface functional groups. **Deconvolution** and second deriv. **spectra** and curve fitting techniques were used to ascertain the frequencies of functional groups. **Samples** after oxidn. by two kinds of **mixed** acid and after redn. in hydrogen were investigated. Exptl. results indicated that several types of carbonyl groups are predominant on the surface of UDD, the contents of which are related to the methods of acid treatment. The main reactions of hydrogen treatment are the conversion of carbonyl groups to hydroxyls, and further to C-H bonding. After reoxidn. of the hydrogen treated samples, the spectra recovered to their original levels, which indicated that redn. reaction of the surface functional groups are reversible.

L6 ANSWER 12 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 124:16286 CA
TI XPS studies on surface species and composition over sulfided K-MoO3/γ-Al2O3 catalysts
AU Bian, Guozhu; Fu, Yilu; Fang, Wenxiu
CS Department Chemical Physics, University Science Technology China, Hefei, 230026, Peop. Rep. China
SO Fenzi Cuihua (1995), 9(5), 329-38
CODEN: FECUEN; ISSN: 1001-3555
PB Zhongguo Kexueyuan Lanzhou Huaxue Wuli Yanjiuso
DT Journal
LA Chinese
AB Two series of sulfided K-MoO3/γ-Al2O3 catalysts with different molybdenum loadings or with different pretreatments before sulfidation were prepd. The relative at. concns. on the surface of the catalysts were measured by XPS. The curve **deconvolution** of XPS **spectra** was used to examine the components of S, Mo spectra and the relative concns. of these species. The results of curve deconvolution show that SO42-, SO3, S0, S22-, MoS2 MoS2-x species in the S spectra and Mo6+, Mo5+, MoS2+x, MoS2, MoS2-x species in the Mo spectra exist on the surface of the samples. For the catalyst with a lower Mo loading [MoO3/Al2O3 (wt. ratio) = 0.03], Mo species are only partly reduced and sulfided during sulfidation. The relative concns. of the MoS2, MoS2-x, Mo6+ components in the Mo spectra show some differences as the Mo loading increases. With Mo loading increased to MoO3/Al2O3 = 0.24, 80% of the Mo species are reduced and sulfided, MoS2, S22- components in the S spectra and MoS2, MoS2-x species in the Mo spectra dominate. For the example with MoO3/γ-Al2O3 wt. ratio of 0.35, ~40% of Mo species are not reduced and sulfided, and about half of the S species exists in S6+ state. The expts. of different pretreatments before sulfidation show that as the oxidized sample comes in contact with water vapor, the structure of the sample is changes remarkably and the molybdenum components become difficult to be reduced and sulfided. The results of activity measurements indicate that the optimum Mo loadings is about MoO3/γ-Al2O3 = 0.24-0.35 for the synthesis of **mixed** alcs. from syngas; and the sulfided **sample** with its precursor contacted with water vapor shows a higher activity. The existence of some higher valence Mo species may be favorable to the synthesis of mixed alcs.

L6 ANSWER 13 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 121:138024 CA
TI Ultraviolet imaging spectrometer for monitoring high-latitude precipitating patterns
AU Mende, Stephen B.; Fuselier, Stephen A.
CS Lockheed Palo Alto Res. Lab., Palo Alto, CA, 94304, USA
SO Optical Engineering (Bellingham, WA, United States) (1993), 32(12), 3139-46
CODEN: OPEGAR; ISSN: 0091-3286
DT Journal
LA English
AB Previously flown satellite imaging expts. have demonstrated the suitability of the VUV region for remote sensing observations of auroral particle pptn. In the wavelength region 120 to 145 nm, a downward-viewing imager is uncontaminated by Earth albedo, and in most cases the intensity of auroral emissions is competitive with rescattered light even during daylit conditions. These features permit quant. imaging of auroral

regions during day and night conditions. An instrument was designed that has adequate wavelength resoln. to sep. key spectral features and simultaneously observe the Doppler profile of the auroral Lyman-α line. This instrument consists of an F3.8 Rowland circle spectrograph with a far-UV intensified CCD at the focal plane. The spectrograph produces a 2-D spectral image where one dimension represents luminosity distribution and the other wavelength dependence. The UV intensified CCD is programmed to pick up the luminosity distribution of various key spectral regions. The entrance slit is parallel to the spin axis and during rotation, a complete luminosity map of the region under the satellite is recorded. The proton velocity distribution will be studied by Doppler profile measurement of the Lyman-α line. A **Hadamard** grille is superimposed on the spectral slit and the Lyman-α data are **deconvolved** to obtain the required wavelength resoln.

L6 ANSWER 14 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 121:124217 CA
TI Application of deconvolution method to the state analysis by EPMA
AU Takahashi, Hideyuki; Okumura, Toyohiko; Seo, Yoshihiro
CS Appl. and Res. Cent., JEOL Ltd., Akishima, 196, Japan
SO X-sen Bunseki no Shinpo (1993), 25, 289-98
CODEN: XBNSDA; ISSN: 0911-7806
DT Journal
LA Japanese
AB X-ray spectra obtained with electron probe micro analyzer (EPMA), which are modified by chem.-bond effect, were **deconvoluted** by using x-ray **spectra** of std. materials. For the deconvolution, the digital filter and the least squares methods were applied, and the obtained results were compared with the ZAF-correction method. In case of SiOx, Si and SiO2 were used as std. materials, and modified Si-Kβ and Si-sKα3,4 **spectra** were **deconvoluted**. The results of quant. anal. coincided well with the results obtained by the application of ZAF-correction method. Thus, it can be said that, when an unknown **specimen** is a **mixt**. of elemental materials, the modified spectrum is a convolution of the spectra of each elemental material. The deconvolution method was also applied to Fe3O4(magnetite) spectrum. In this case, Fe3O4 was assumed as an unknown material, and FeO(wustite) and Fe2O3(hematite) were taken as the std. materials. The results from Fe-Lα and Fe-Lβ coincided well with the result from the ZAF-correction method, but the result from O-Kα did not. It was found that materials with the same crystal structure give similar O-Kα spectra but those with different crystal structures give different O-Kα spectra. This fact shows that the O-Kα spectrum from Fe3O4(spinel type) is not identified as the convolution of those from FeO(NaCl type) and Fe2O3(corundum type). The disagreement between the result from the deconvolution method and that from the ZAF-correction method is due to the above reason. On the other hand, Fe-Lα and -Lβ spectra are influenced mainly by the outer electron distribution and charge balance in the constituted atoms, but not by the crystal structure difference. Therefore, they coincide well with the convolution of spectra due to those of FeO and Fe2O3.

L6 ANSWER 15 OF 25 CA COPYRIGHT 2003 ACS on STN
Full Text
AN 120:275892 CA
TI Ultraviolet imaging spectrometer [UVIS] for monitoring high latitude precipitating patterns
AU Mende, S. B.; Fuselier, S.; Jamar, C.

CS Lockheed Palo Alto Res. Lab., Palo Alto, CA, 94304, USA
SO Proceedings of SPIE-The International Society for Optical Engineering (1993), 2008(Instrumentation for Magnetospheric Imagery II), 173-82
CODEN: PSISDG; ISSN: 0277-786X
DT Journal
LA English
AB Previously flown satellite imaging expts. have demonstrated the suitability of the vacuum UV region for remote sensing observations of auroral particle pptn. In the wavelength region 120-145 nm, a downward viewing imager is uncontaminated by the earth albedo and the intensity of the auroral emissions in most cases is competitive with the rescattered light even during daylit conditions. These features permit the quant. imaging of the auroral regions during day and night conditions. An instrument suitable for such observation which has adequate wavelength resoln. to sep. key spectral features and simultaneously obsd. the Doppler profile of the auroral Lyman alpha line was designed. This instrument, in its simplest form, consists of an F3.8 Rowland circle spectrograph with an FUV intensified CCD at the focal region. The entrance slit is perpendicular to the orbit plane and parallel to the spin axis of the satellite. The field of view of the instantaneous slit image is 50° in the direction perpendicular to the rotational axis and 1° parallel to the spin axis [i.e. in the direction parallel to the orbital plane]. The spectrograph produces a two dimensional spectral image where one dimension represents luminosity distribution and the other wavelength dependence. The UV intensified CCD is programmed to pick up the luminosity distribution of various key spectral regions. During the 360° rotation, a complete luminosity map of the 50° wide region under the satellite is recorded. Depending on the satellite rotation rate and the wavelength of interest, more than one complete rotation will be needed to achieve the desired signal to noise ratio. The proton velocity distribution will be studied by high spectral resoln. Doppler profile measurement of the Lyman alpha line. This is accomplished through the subdivision of the entrance slit into a set of smaller parallel slits representing a mask of a **Hadamard** S matrix type and the Lyman alpha data is **deconvolved** to obtain the required wavelength resoln.

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Full Text
AN 120:163237 CA
TI Photofragmentation in Fourier-transform ion cyclotron resonance: use or misuse?
AU Gaumann, Tino; Zhao, Guohong; Zhu, Zhiqing
CS Phys. Inst., Federal Sch. Technol., Lausanne, Switz.
SO Rapid Communications in Mass Spectrometry (1994), 8(1), 1-9
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DT Journal
LA English
AB The noise in a sector or quadrupole mass spectrometer is detd. by the source, i.e. the no. of ions present in the signal, whereas in Fourier-transform ion cyclotron resonance it is detector limited. In addn., the Fourier transform spreads white noise equally over the whole spectrum. Thus the accuracy for broad-band spectra is generally rather low. However, the precision, i.e. the reproducibility of successive spectra, is astonishingly high. This fact has been used with much success, for example in collisionally activated dissocn. in **Hadamard** spectra. It is shown that photofragmentation spectra are also very reproducible and thus allow - at least in principle - a 'kinetic **deconvolution**' of a series of such spectra. In such a case, nonlinear regression has to be applied to the data. Since in most kinetics problems several exponential functions are involved, and since it is well known